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# Intermediate Neglect of Differential Overlap Calculations on the Electronic Spectra of Transition Metal Complexes

by

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To Appear as a Back Chapter in a
NATO ASI on Metal-Ligand Interactions

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# Intermediate Neglect of Differential Overlap Calculations on the Electronic Spectra of Transition Metal Complexes

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## 1. Introduction:

The title of this manuscript really suggests three separate subjects:(1) The Intermediate Neglect of Differential Overlap Model (INDO/S) that we have used for many years to describe the electronic spectra and photochemistry of large systems, (2) the description of how one might calculate electronic spectroscopy, and finally, (3) the electronic structure of transition metal complexes, *per se*. I should like to begin with the third of these, which is the theme of this school, paying only cursory attention to the first two. Transition metal compounds *are* different from compounds that contain only main group elements, and I think it is interesting to examine *why*. After all, there are rather good computational tools for examining the electronic structure of molecules that do not contain transition metal compounds that are now widely used by theorists and experimentalists alike. So called *ab-initio* programs such as Gaussian92[1], GAMESS[2], Turbomole[3], ACESII[4], are rather sophisticated packages that yield accurate results for smaller systems, AMPAC[5], MOPAC[6], ZINDO[7] and SINDO[8] are semi-empirical methods available for rather large systems, and there are molecular modeling methods that use classical force fields such as AMBER[9], CHARM[10] and INSIGHT[11] that can be used for thousands of atoms. Such programs have not been widely used in the study of transition metal compounds. Why is that?

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